

# Spin-resolved electron-impact ionization of lithium

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**Abstract.** Electron-impact ionization of lithium is studied using the convergent close-coupling (CCC) method at 25.4 and 54.4 eV. Particular attention is paid to the spin-dependence of the ionization cross sections. Convergence is found to be more rapid for the spin asymmetries than for the underlying cross sections. Comparison with the recently measured and DS3C-calculated data of Streun *et al* (1999) is most intriguing. Excellent agreement is found with the measured and calculated spin asymmetries, yet the discrepancy between the CCC and DS3C cross sections is very large.

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## 1. Introduction

One of the great strengths of the field of electron-atom scattering is the strong interplay between theory and experiment. Generally, experiment is used to test theory and so leads the way forward. The ultimate goal of a measurement of a particular scattering process is to perform a so-called complete experiment, one that fully determines all possible aspects of the collision (Bederson 1969*a*, Bederson 1969*b*). Such measurements are able to fully test the scattering amplitudes arising in any theory. In practice this goal has been rarely achieved, with electron-impact excitation of the  $nP$  states of helium being a notable example (see Fursa and Bray (1995) and references therein). However, this scattering process is not particularly rich in information requiring the measurement, at each scattering angle, of only the differential cross section and the three Stokes parameters to fully test the two independent theoretical (complex) scattering amplitudes. One way to increase the scattering process information is to scatter electrons from a non-spin-zero atomic target. This immediately doubles the number of scattering amplitudes, and allows for a thorough test of the theoretical treatment of electron-exchange processes. It was electron scattering on the H and Na targets which showed the accuracy of the convergent close-coupling (CCC) approach to electron-atom scattering (Bray and Stelbovics 1993, Bray 1994*c*).

Another way to increase the amount of information associated with a scattering process is to consider excitation of more complicated final states or, at energies above the ionization threshold, to measure the fully resolved differential ionization (e,2e) cross sections. Though initially the close-coupling approach has been applied to elastic and discrete excitation processes, it has been clear for some time that intermediate excitation of the continuum must be treated in order to ensure accurate final results. The CCC method has proved particularly successful in this regard and showed that e-Na spin-resolved 3P excitation description required detailed coupling within the continuum (Bray 1994*b*). This unexpected result encouraged us to look directly at ionization processes.

The CCC application to electron-impact ionization of helium has been particularly successful for asymmetric (Bray and Fursa 1996, Röder *et al* 1996*a*, Röder *et al* 1996*b*) and equal-energy sharing (Bray *et al* 1997, Bray *et al* 1998, Rioual *et al* 1998) kinematics. Some problems with absolute values were identified (Röder *et al* 1997) and explained by reference to the mechanics of the close-coupling method (Bray 1997). While the total ionization cross section (TICS) is very stable at all energies as a function of the number of states  $N$  used to expand the total wave function, the underlying singly differential ionization cross section (SDCS) may not be. The TICS is stable due to the unitarity of the formalism, which does not allow for any double-counting of the ionization cross sections even though these are obtained from excitation of pseudostates of positive energy  $0 < \epsilon_n^{(N)} < E$  where  $E$  is the total (excess) energy. We believe the instability in the SDCS is due to convergence to zero of excitation amplitudes of states with  $E/2 < \epsilon_n^{(N)} < E$ . This leads to a step-function SDCS. Though this explanation has

been met with some hostility (Bencze and Chandler 1999), who claim that the CCC-calculated SDCS should instead be symmetric about  $E/2$  (at odds with unitarity!) we are still confident that our interpretation is correct (Bray 1999b), and enhanced by the work of Stelbovics (1999). Whereas we supposed that the CCC amplitudes at the step would converge extremely slowly in magnitude to the full size of the step, Stelbovics (1999) showed, in effect, that the CCC amplitudes have converged, but to half the step size. His analysis reconciles the coherent versus incoherent combination of the amplitudes at  $E/2$ , see discussion by Bray (1999a). Furthermore, other approaches have shown consistency and accuracy of the CCC method (Miyashita *et al* 1999, Baertschy *et al* 1999).

What we find more disturbing is that a systematic application of the CCC method to e-H ionization has shown inconsistent agreement with experiment (Bray 1999a). In the energy region between 17.6 and 30 eV there is at times substantial disagreement with experiment, not found in the e-He case. The e-H and e-He ionization problems differ in that the former needs to be solved for two total spins. This may cause the CCC method more difficulty in treating targets like H as opposed to He. Having spin-resolved fully differential e-H ionization measurements would be particularly helpful. Unfortunately, this has not yet occurred, but there has been substantial progress in measuring closely related e-Li ionization processes (Baum *et al* 1992, Streun *et al* 1998, Streun *et al* 1999).

The aim of this paper is to examine the implications of the analysis of Stelbovics (1999) on spin-resolved cross sections in the case of 54.4 eV e-Li ionization. In addition, we compare the CCC method with the recent measurements and calculations of e-Li ionization at 25.4 eV by Streun *et al* (1999).

## 2. Theory

The details of the CCC theory for ionization of atoms by electron impact have been given by Bray and Fursa (1996). This was suitable for hydrogen and helium targets with extension to lithium being trivial using the details given by Bray (1994c). Briefly, the structure of the lithium atom is obtained by diagonalising the target frozen-core Hartree-Fock Hamiltonian  $H_2$  using an orthogonal (one-electron) Laguerre basis. This is possible after the core 1s wave function has been evaluated using the self-consistent field Hartree-Fock equations. Upon diagonalisation  $n = 1, \dots, N$  square-integrable target states  $\phi_n^{(N)}$  with energies  $\epsilon_n^{(N)}$  are obtained. The negative-energy states describe the discrete spectrum, while the positive-energy states provide a discretization of the target continuum. For a given incident electron energy  $k_i^2/2$  the close-coupling equations are solved for the  $T$  matrix, separately for each total spin  $S$ , to define the scattering amplitudes for excitation of states  $\phi_f^{(N)}$  of energy  $\epsilon_f^{(N)} < E$

$$f_S^{(N)}(\mathbf{k}_f, \mathbf{k}_i) \equiv \langle \mathbf{k}_f(1) \phi_f^{(N)}(2) | T_S | \phi_i^{(N)}(2) \mathbf{k}_i(1) \rangle, \quad (1)$$

where  $E = k_i^2/2 + \epsilon_i^{(N)}$  is the total (excess) energy, and where the numbers in parenthesis indicate electron space.

Thus, the problem looks as if only discrete excitation has been treated. We associate ionization with excitation of the positive-energy states. Assuming that the asymptotic Hamiltonian may be partitioned asymmetrically as  $K_1 + H_2$ , where  $K_1$  is the projectile-space kinetic energy operator, leads to the definition of the (e,2e) amplitude

$$f_S^{(N)}(\mathbf{k}_f, \mathbf{q}_f, \mathbf{k}_i) \equiv \langle \mathbf{q}_f^{(-)} | \phi_f^{(N)} \rangle \langle \mathbf{k}_f \phi_f^{(N)} | T_S | \phi_i^{(N)} \mathbf{k}_i \rangle, \quad (2)$$

where  $\langle \mathbf{q}_f^{(-)} |$  is a continuum eigenstate of  $H_2$  of energy  $q_f^2/2 = \epsilon_f^{(N)}$  (Bray and Fursa 1996).

The fundamental problem with the application of the close-coupling approach to ionization is that allowance for excitation of states with  $0 < \epsilon_f^{(N)} < E$ , equivalent to integration over the continuum from 0 to  $E$ , suggests double-counting of ionization processes. Yet being a unitary theory, which yields accurate total ionization cross sections (TICS) (Bray and Stelbovics 1993), is a contradiction to this. The step-function idea (Bray 1997), suggested upon numerical investigation, says that with increasing  $N$  the amplitudes for excitation of states with  $E/2 < \epsilon_f^{(N)} < E$  will converge to zero, with the resulting secondary energy integration being from 0 to  $E/2$  as in formal theory of ionization. The question remains as to how to define the cross sections for finite  $N$ . The incoherent combination of amplitudes on either side of  $E/2$ ,

$$\frac{d^3 \sigma_S^{(N)}}{d\Omega_1 d\Omega_2 dE_2} = |f_S^{(N)}(\mathbf{k}_f, \mathbf{q}_f, \mathbf{k}_i)|^2 + |f_S^{(N)}(\mathbf{q}_f, \mathbf{k}_f, \mathbf{k}_i)|^2, \quad (3)$$

was suggested by Bray and Fursa (1996) as a way of preserving unitarity. This combination had nothing to do with Pauli symmetrization, only aimed at preserving the accuracy of the TICS for the energy integration ending at  $E/2$ . The individual  $f_S$  are already a coherent combination of their own direct and exchange amplitudes. The second term must not be confused with an “exchange” term. It is a numerical “double-counting” term which should be near zero for  $q_f < k_f$ . Typically, the term with  $q_f < k_f$  is by far the most dominant. Only at  $E/2$  are the two terms quite similar.

While (3) yielded excellent angular distributions the magnitude of the  $E/2$  cross sections was typically around a factor of two too low (Bray *et al* 1997, Bray *et al* 1998, Rioual *et al* 1998). We put this down to extremely slow convergence of amplitudes to the top of the step size. Stelbovics (1999) analysed the close-coupling approach to ionization in a model e-H problem and concluded that at  $E/2$  the cross section should be defined as

$$\frac{d^3 \sigma_S^{(N)}}{d\Omega_1 d\Omega_2 dE_2} = |f_S^{(N)}(\mathbf{k}_f, \mathbf{q}_f, \mathbf{k}_i) + (-1)^S f_S^{(N)}(\mathbf{q}_f, \mathbf{k}_f, \mathbf{k}_i)|^2, \quad (4)$$

and that the CCC amplitudes at  $E/2$  had converged but to half the step size, as if solving the CCC equations is like performing Fourier expansions of step functions. Hence (3) should be multiplied by exactly two, but only for the case of equal energy-sharing, and hence not affecting the accuracy to which unitarity is satisfied. For asymmetric energy sharing Stelbovics (1999) showed that only if the CCC amplitudes were identically zero in the energy range  $E/2 < \epsilon_f^{(N)} < E$  could the ionization amplitudes

be unambiguously defined. In which case they are just the CCC amplitudes in the energy region  $0 < \epsilon_f^{(N)} \leq E/2$ . For practical purposes he suggested that the error with using (4) generally would be relatively small.

At first glance one might expect substantial difference between (4) and (3). For substantially asymmetric energy sharing  $q_f < k_f$  only the first term contributes significantly, and so both prescriptions give a similar result. At  $E/2$  we need to multiply (3) by two before comparison with (4). A detailed numerical comparison for e-H ionization has been given (Bray 1999a) and found that the two forms were barely distinguishable. The reason for this is that if  $q_f = k_f$  then

$$f_S^{(N)}(\mathbf{k}_f, \mathbf{q}_f, \mathbf{k}_i) = (-1)^S f_S^{(N)}(\mathbf{q}_f, \mathbf{k}_f, \mathbf{k}_i) + \delta_S^{(N)}(\mathbf{k}_f, \mathbf{q}_f, \mathbf{k}_i), \quad (5)$$

where  $\delta_S^{(N)}$  is a relatively small number in practical calculations, which should converge to zero with increasing  $N$ . The difference between  $2 \times (3)$  and (4) is  $|\delta_S^{(N)}|^2$ . This reconciles the two approaches and yields similar results in realistic e-H calculations. We should mention that the problem with lack of convergence in the magnitudes of the CCC amplitudes at asymmetric energy-sharing remains and we resort to a semi-empirical rescaling of these amplitudes utilising the known values at  $E/2$  (Bray 1999a).

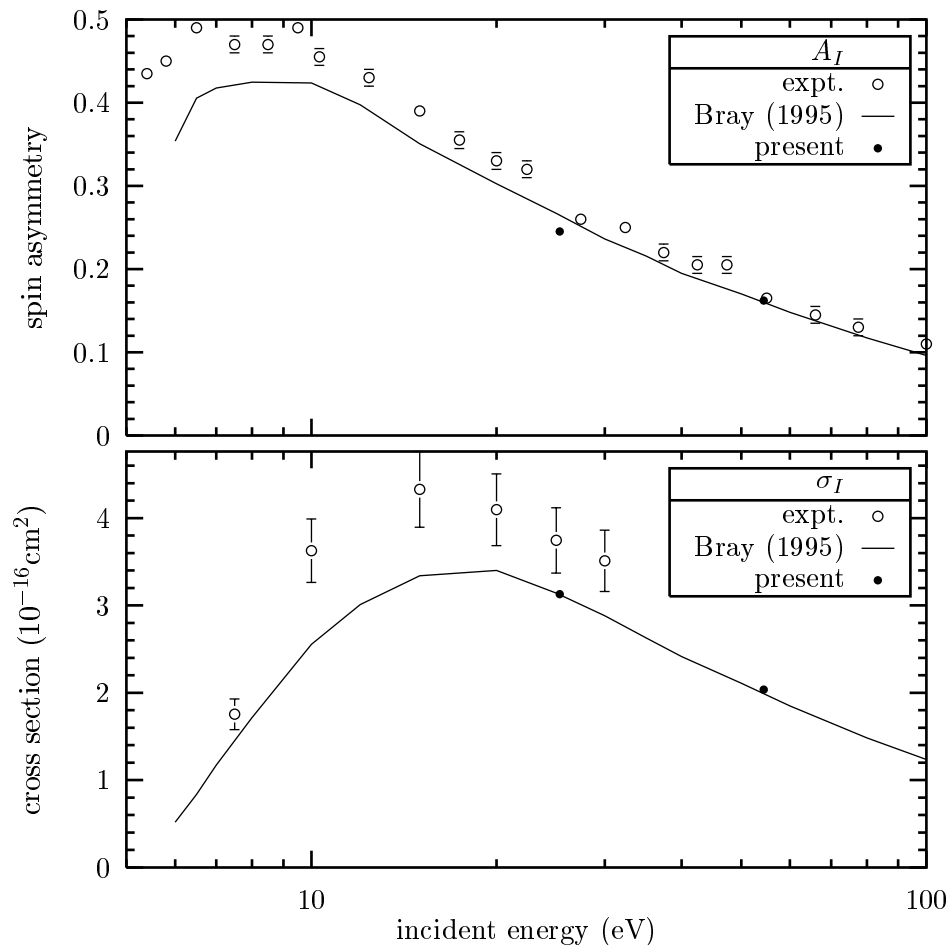
### 3. Results

Before looking at the detailed results for the two incident electron energies considered we present, in figure 1, the total ionization cross sections and their spin asymmetries. These are compared with previous, much smaller, CCC calculations and experiment. Good agreement is found of the present calculations with the old for both parameters. Agreement with the spin asymmetry measurements is satisfactory given the stated systematic uncertainty (Baum *et al* 1985). Convergence for the cross section is very good, and thus the systematic discrepancy with the measurements of Zapesochnyi and Aleksakhin (1969) persists.

#### 3.1. Electron-lithium ionization at 54.4 eV

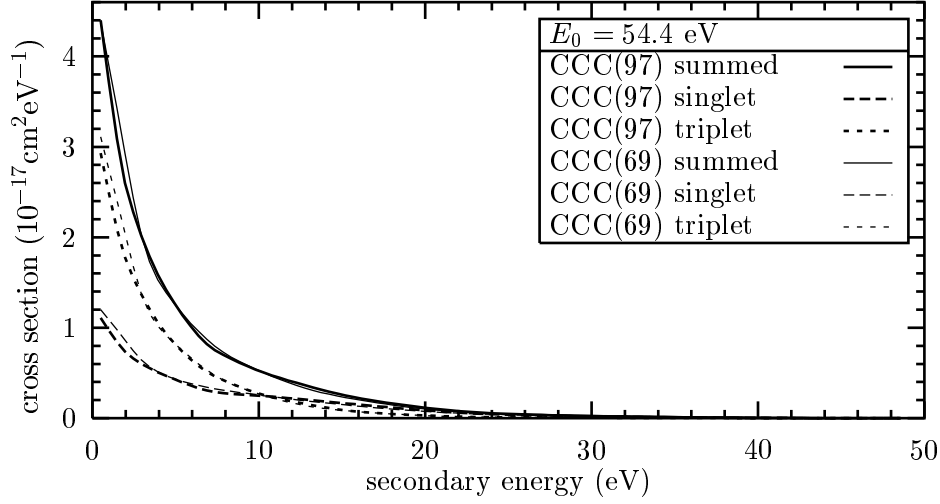
Experimental data for e-Li ionization is available for 54.4 eV incident energy ( $E = 49$  eV), with secondary electrons having energy (eV) sharing as  $(E_B, E_A)$  pairs of (5,44), (14,35) and (24.5,24.5) (Streun *et al* 1998). A CCC(69) calculation has already been presented for these cases by Streun *et al* (1998). Here we also give a CCC(97) calculation which has maximum target-space orbital angular momentum  $l_{\max} = 6$  with around 18- $l$  states for each  $l$ . The 69-state calculation has  $l_{\max} = 5$  with around 15- $l$  states for each  $l$ . The 97-state calculation requires approximately 1.5 G of RAM. In addition to checking convergence in both the spin asymmetries and differential cross sections, for the (24.5,24.5) case we also consider the generation of these using both the combinations (3) multiplied by two and (4).

In figure 2 we compare the SDCS arising in the 69- and 97-state calculations. We see that both the singlet and triplet components are rather smooth and fall-off to zero



**Figure 1.** Total ionization cross sections and spin asymmetries for electron-impact ionization of the ground state of lithium. The results of the two present calculations are indicated by the solid dots. The spin asymmetry experimental data are due to Baum *et al* (1985) and the total ionization data are due to Zapesochnyi and Aleksakhin (1969). The solid curve is due to CCC calculations reported by Bray (1995).

uniformly. In experiment the SDCS would be measured to be symmetric about 24.5 eV, and the present results should not be viewed as a contradiction to this, as Bencze and Chandler (1999) have. What is plotted is the square of the magnitude of the amplitude (2) integrated over the angles of the outgoing electrons. If we were to use the form (3) or (4) an almost identical symmetric SDCS would result, with the difference that (4) would yield a cross section two times bigger at the secondary energy of 24.5 eV. The plotted SDCS yield TICS upon secondary energy integration from 0 to  $E$ , whereas the symmetric forms would have  $E/2$  as the endpoint of integration. It is the smallness of the cross section at 24.5 eV that, in our view, allows the CCC method to yield relatively accurate SDCS at the smaller secondary energies. In other words, the step-function is relatively easy to satisfy for the 54.4 eV incident energy, and all of the possible physical processes are treated by the pseudostates with  $\epsilon_f^{(N)} \leq E/2$ .



**Figure 2.** The singly differential cross section for 54.4 eV electron-impact ionization of the ground state of lithium calculated using the 69- and 97-state approximations. The singlet and triplet cross sections include the spin weights.

The spin-averaged triply differential cross sections (TDCS) is

$$\frac{d^3\sigma^{(N)}}{d\Omega_1 d\Omega_2 dE_2} = \frac{1}{4} \frac{d^3\sigma_{S=0}^{(N)}}{d\Omega_1 d\Omega_2 dE_2} + \frac{3}{4} \frac{d^3\sigma_{S=1}^{(N)}}{d\Omega_1 d\Omega_2 dE_2}, \quad (6)$$

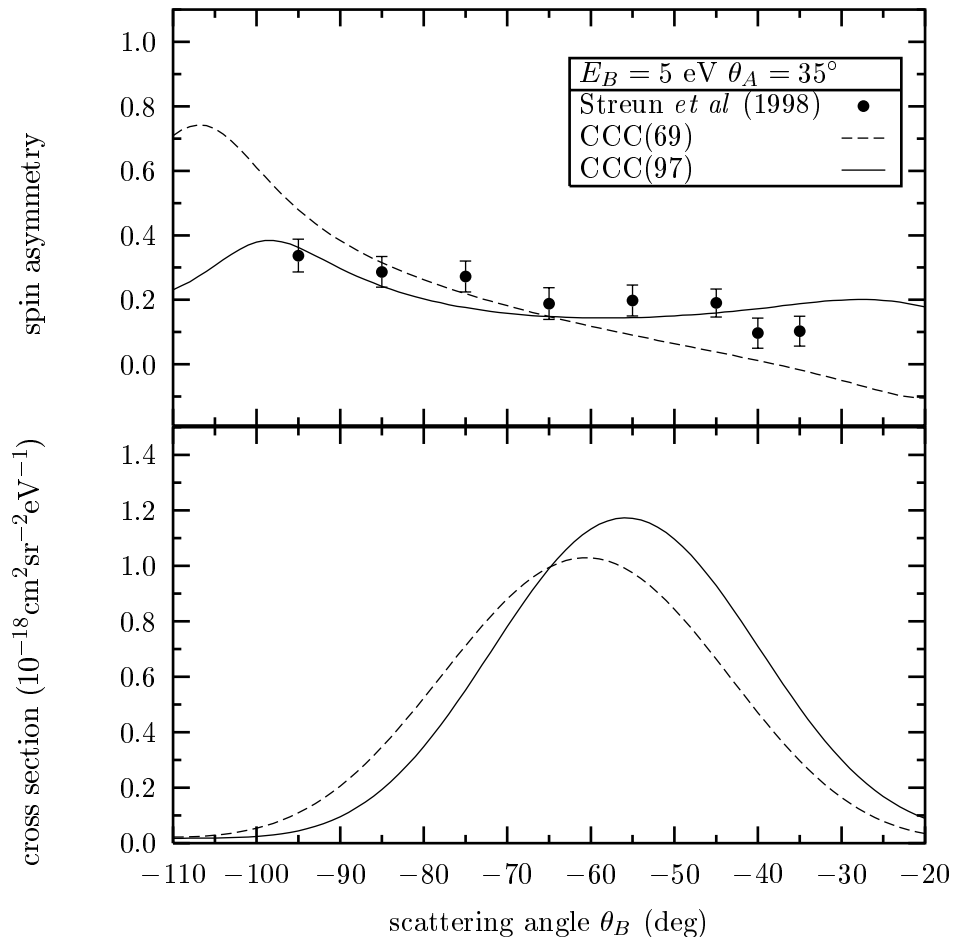
and the corresponding spin asymmetry is

$$A = (1 - r)/(1 + 3r), \quad (7)$$

where  $r$  is the ratio of the triplet to singlet (no spin weights) TDCS. These are given for the secondary energy of  $E_B = 5$  eV in figure 3 in the geometry where the fast (44 eV) electron is detected at  $\theta_A = 35^\circ$ . We use the notation, convenient in the coplanar geometry, that negative angles are on the opposite side of the incident beam ( $z$ -axis) to the positive angles. We see that there is some difference between the two calculations with the asymmetry varying more where the cross section is small. This is an example of the general statement that the smaller the cross section the bigger the calculation necessary to obtain such cross sections accurately. Further, even larger calculations, which grow very rapidly with increasing  $l_{\max}$ , would be necessary to determine the cross sections more accurately. Nevertheless agreement with experiment is satisfactory for both the spin asymmetries, and is superior to the distorted wave Born approximation (DWBA) reported by Streun *et al* (1998).

Figure 4 reports results for the  $E_B = 14$  eV case. Somewhat better convergence is found for this case for both the spin asymmetries and the TDCS. Agreement with experiment is good and is of the same quality to that of the DWBA calculation reported by Streun *et al* (1998).

The equal-energy sharing case  $E_B = E_A = 24.5$  eV presented in figure 5 is more interesting. For the two previous cases combinations (3) and (4) yield near identical results due to the second “double-counting” term being negligible, see figure 2 for energies greater than 24.5 eV. However, at equal energy-sharing both terms come

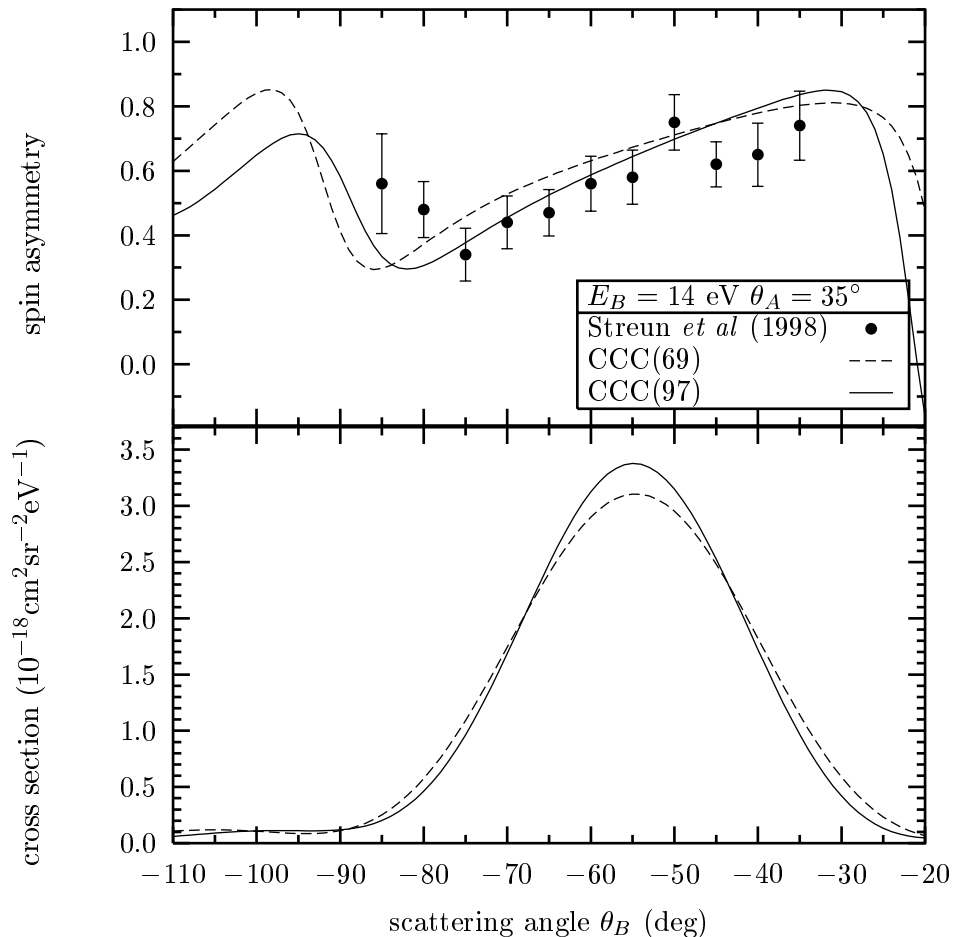


**Figure 3.** The coplanar  $\theta_A = 35^\circ$ ,  $E_B = 5$  eV triply differential cross section and spin asymmetry for 54.4 eV electron-impact ionization of the ground state of lithium calculated using the 69- and 97-state approximations. The measurements and the CCC(69) calculation have been reported by Streun *et al* (1998).

into play as they are derived from the same amplitudes (2). Due to the suggestion of Stelbovics (1999) that at  $E/2$  the CCC amplitudes converge to half the step size, the results of (3) need to be multiplied by two before comparison with (4), which only affects the TDCS and not the spin asymmetries.

Let us examine the TDCS first. Around the maximum of the TDCS both forms give much the same result, which differ substantially for the two calculations. The difference between the CCC(69) and CCC(97) curves is not surprising, and is primarily due to the increase by one of  $l_{\max}$  in the latter calculation. Given that the outgoing electron energies are 24.5 eV one would expect to require even substantially larger than  $l_{\max} = 6$ . However, the unitarity of the close-coupling formalism severely restricts flux to large angular momentum channels as this is related to convergence in just the elastic scattering channel (Bray 1994a). The agreement between the two combinations of amplitudes for the larger TDCS indicates that  $\delta_S^{(N)}$  in (5) is relatively small at those angles. Thus, we see that while satisfying (5) is a good thing, the difference between the CCC(97) and CCC(69) TDCS indicates that it is not sufficient to assure accuracy

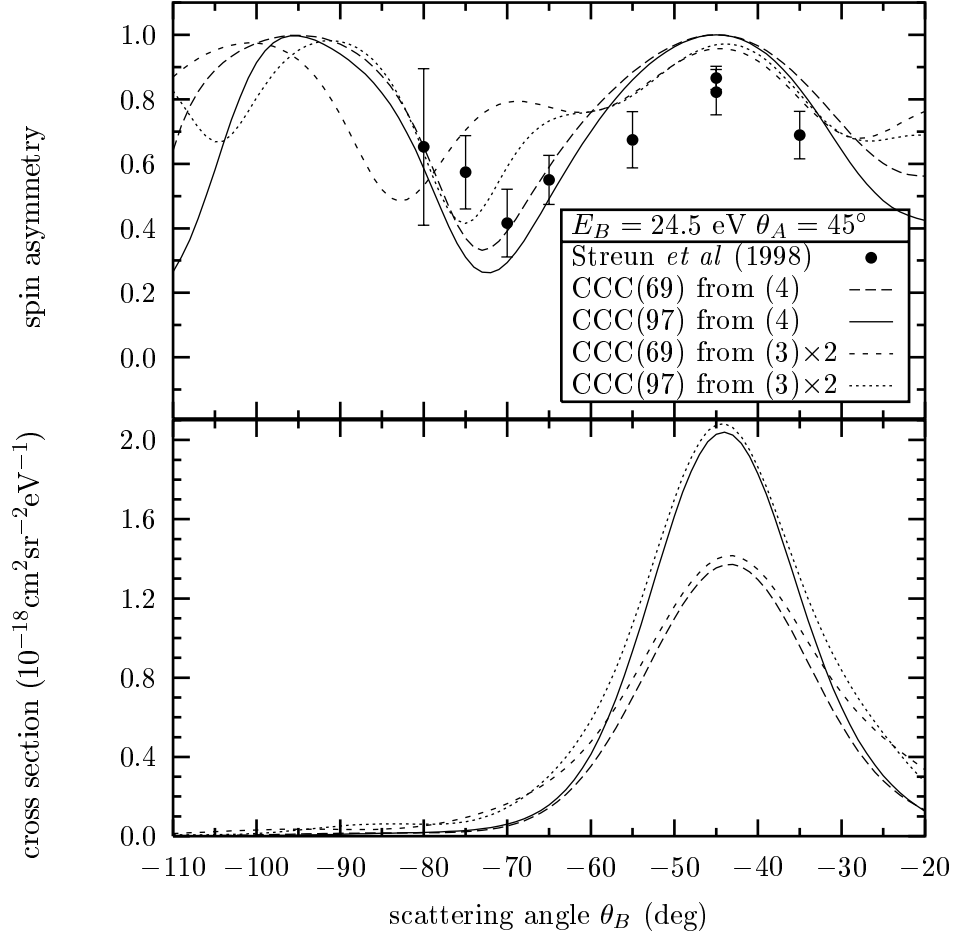




**Figure 4.** The coplanar  $\theta_A = 35^\circ$ ,  $E_B = 14 \text{ eV}$  triply differential cross section and spin asymmetry for 54.4 eV electron-impact ionization of the ground state of lithium calculated using the 69- and 97-state approximations. The measurements and the CCC(69) calculation have been reported by Streun *et al* (1998).

of the results. Clearly calculations with even larger  $l_{\text{max}}$  are necessary to obtain a more accurate estimate of the TDCS.

Turning our attention to the spin asymmetries, we see that the form (4) yields identically unity for the  $\theta_A = -\theta_B = 45^\circ$  case. This is expected from the Pauli Principle with the triplet TDCS vanishing identically in (4) and almost so in (3) due to (5). What is particularly interesting is that (4) yield much closer results for the two CCC calculations than does (3). Most encouraging is the removal, by the use of (4) instead of (3), of the oscillation around  $\theta_B = -70^\circ$ , not seen in experiment or the DWBA theory (Streun *et al* 1998). This means that the combination (4) is more efficient at hiding a lack of convergence in the underlying CCC amplitudes by the construction of the exactly required symmetry in the amplitudes used to generate the TDCS.

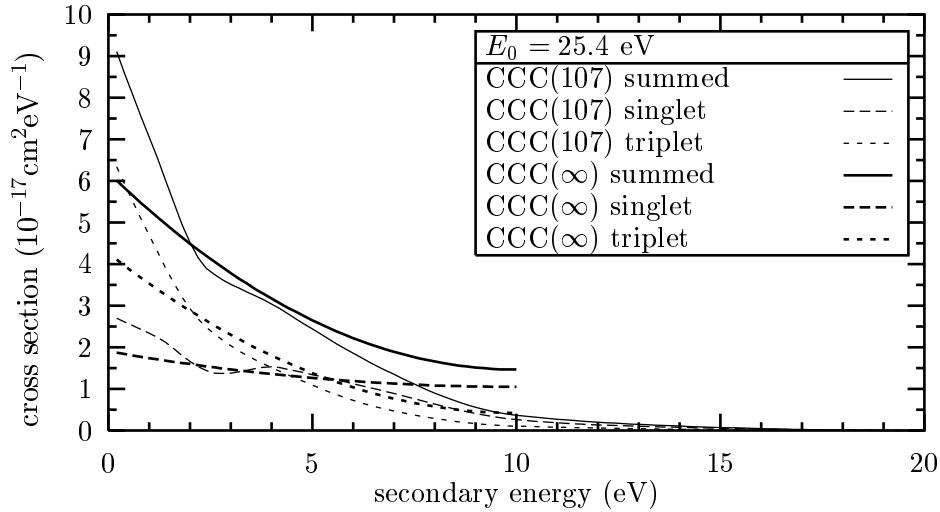


**Figure 5.** The coplanar  $\theta_A = 45^\circ$ ,  $E_B = 24.5$  eV triply differential cross section and spin asymmetry for 54.4 eV electron-impact ionization of the ground state of lithium calculated using the 69- and 97-state approximations. The cross sections and the spin asymmetries have been calculated using (3) and (4). The measurements and the CCC(69) calculation have been reported by Streun *et al* (1998).

### 3.2. Electron-lithium ionization at 25.4 eV

The recent measurements of Streun *et al* (1999) at 25.4 eV incident energy ( $E = 20$  eV) take a different form to those above. The coplanar symmetric  $\theta_A = -\theta_B = 45^\circ$  single point is taken, and the asymmetry measured at this point as a function of the energy-sharing of the two electrons. Given the difficulty the CCC theory has in obtaining convergent SDCS at low energies, such measurements are particularly challenging for the theory.

We present the results of just a single CCC calculation, which has been checked for convergence. It couples a total of 107 states, where  $l_{max} = 7$  and has around 18- $l$  states for each  $l$ . The Laguerre exponential fall-offs  $\lambda_l \approx 2$  were varied slightly to ensure a pseudostate of 10 eV for each  $l$  resulting with a total of around ten other positive-energy states. The amplitudes for arbitrary  $E_B$  are obtained by interpolation (Bray and Fursa 1996).

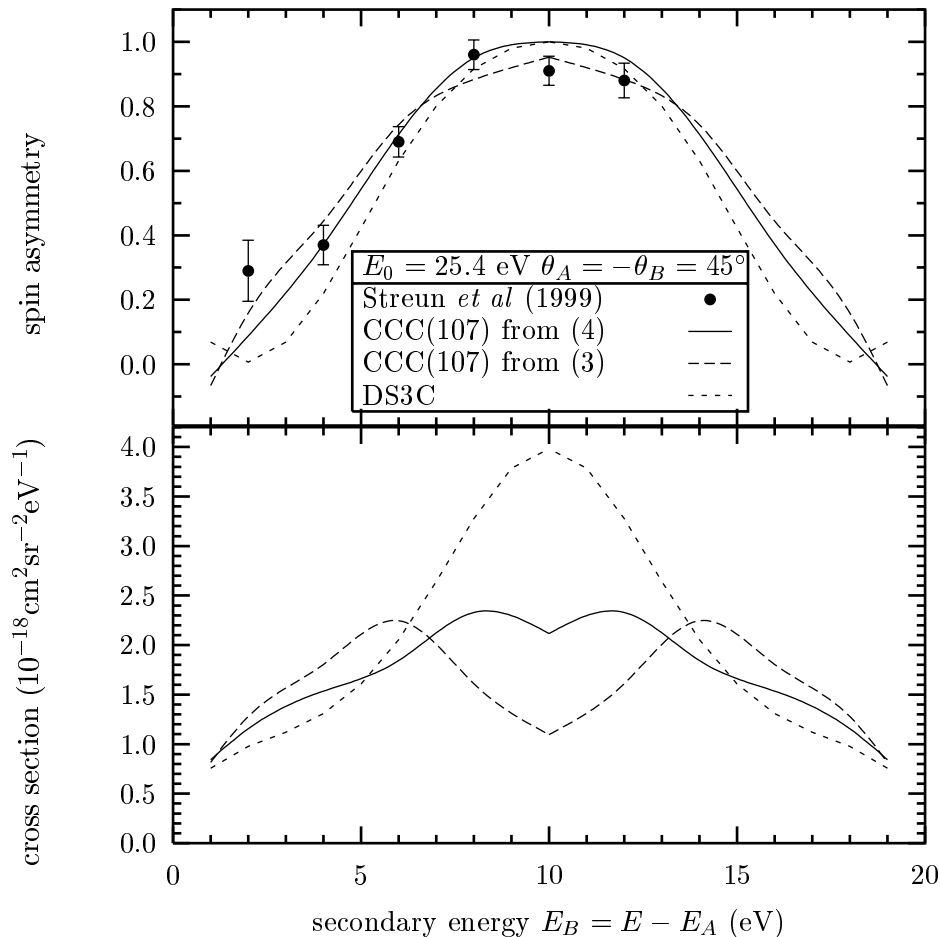


**Figure 6.** The singly differential cross section for 25.4 eV electron-impact ionization of the ground state of lithium calculated using the 107-state CCC calculation. Also given are integral preserving estimates labelled by CCC( $\infty$ ), see text. The singlet and triplet cross sections include the spin weights.

Firstly, in figure 6, the SDCS are given. We see that the individual CCC(107) singlet and triplet SDCS have unphysical oscillations. These are due to, we suspect, the SDCS( $E/2$ ) being substantial. Also given are the quadratic integral preserving estimates, labelled as CCC( $\infty$ ), whose SDCS( $E/2$ ) are four times the CCC(107) SDCS( $E/2$ ). The label  $\infty$  is used to suggest the result of a fully convergent close-coupling calculation. Note that at  $E/2$  the convergence of CCC( $\infty$ ) is to CCC(107) SDCS( $E/2$ ), that is a quarter of the step size owing to convergence of CCC(107) amplitudes to half the true amplitude at  $E/2$ .

There is quite substantial difference between the CCC( $\infty$ ) and CCC(107) curves, not only around  $E/2$  but also at small secondary energies. While we do not know how accurate the CCC( $\infty$ ) estimates are we believe them to be more accurate than the CCC(107) raw results and would use them to rescale the magnitudes of any TDCS calculated for  $E_B < E/2$ .

Figure 7 gives the CCC(107) spin asymmetries and TDCS corresponding to the experiment and calculations of Streun *et al* (1999). Turning our attention to the spin asymmetries we see very good agreement between the CCC(107) calculation, using (3) and (4), the DS3C calculation, and the experiment. The agreement between the use of (4) and DS3C is a little better than the use of (3). This is particularly evident around  $E/2$  where both yield exactly unity, as would be expected. The discrepancy with experiment in this case is due to experimental uncertainties. One may ask what effect would rescaling the CCC calculations according to the CCC( $\infty$ ) estimates given in figure 6. For the  $E_B = 2$  eV no change would result as here the estimates and the raw results intersect. At  $E_B = 4$  eV the estimates suggest a small increase in the triplet component and a small decrease in the singlet component. This would result in



**Figure 7.** The coplanar  $\theta_A = -\theta_B = 45^\circ$  triply differential cross section and spin asymmetry for 25.4 eV electron-impact ionization of the ground state of lithium calculated using the 107-state CCC calculation for both Eqs.(3) and (4). Also given are the DS3C results of Streun *et al* (1999).

a decrease in the asymmetry (see (7)), and hence the DS3C calculation is perhaps more accurate here, even though the relevant CCC result goes through the midpoint of the error bar. At  $E_B = 6$  eV the estimates predict a drop in the triplet cross section and therefore a further small rise in the asymmetry. Lastly, for  $E_B = 8$  eV both the singlet and triplet cross sections estimates are twice the raw results, unaffected the asymmetry.

The good agreement between the theories for the spin asymmetry is lost when the corresponding TDCS is considered. The factor of two difference at  $E/2$  between the CCC(107) results evaluated using (3) and (4) is expected. Thus there is no way for (3) to yield accurate SDCS in the vicinity of  $E/2$ . The question is how accurate is the coherent combination (4)? While we are confident of the accuracy of the magnitude yielded by (4) at  $E/2$ , which is considerably lower than that predicted by the DS3C theory, the cusp here looks somewhat unphysical. Given that detailed convergence studies in a model problem show an ever increasing slope of the CCC-calculated SDCS at  $E/2$  (Bray 1997), even the new form (4) may be unable to achieve accuracy in the SDCS in a neighbourhood of  $E/2$ , even while having convergent SDCS at  $E/2$ .

Another interesting feature that arises from the consideration of the TDCS is the visible difference between the usage of (3) and (4) for the asymmetric energy sharing below 5 eV. This is surprising given the SDCS presented in figure 6. The reason for the difference is simple. If we write the ratio of the presented SDCS(15)/SDCS(5) =  $r^2$ , then the ratio of the corresponding amplitudes is just  $r$ . Since the combination (3) sums cross sections, the contributions past  $E/2$  only significantly contribute to the presented TDCS in the energy region 5 to 15 eV. However, the combination (4) has CCC amplitudes calculated at energies greater than  $E/2$  contributing visibly to the presented TDCS over a much wider energy range.

Unfortunately, the difference between the two CCC-calculated TDCS is somewhat academic since the underlying amplitudes have only converged to an acceptable accuracy at the  $E/2$  point. The difference between the estimated and calculated SDCS in figure 6 is indicative of the lack of convergence (except at the  $E/2$  point). Hence rescaling the CCC-calculated TDCS utilising the SDCS estimates would probably result in TDCS more accurate than those presented.

#### 4. Conclusions

Spin-resolved electron-lithium ionization TDCS have been considered for the 54.4 and 25.4 eV incident energies. For both cases asymmetric through to symmetric energy-sharing kinematics were considered. At the higher energy reasonable convergence in the spin asymmetries has been achieved and good agreement with available experiment obtained in all cases. For the equal energy-case the combination of amplitudes suggested by Stelbovics (1999), see (4), yields more accurate spin asymmetries. This indicates that obtaining convergent underlying CCC amplitudes of correct symmetry is more difficult in the case of lithium than for atomic hydrogen (Bray 1999a). The explicit imposition of the required symmetry via (4) allows for a faster rate of convergence in observable phenomena.

At the lower energy the SDCS at  $E/2$  is relatively more substantial than at the higher energy and therefore the convergence in the CCC ionization amplitudes has not been achieved generally. Numerically, it is too difficult to adequately reproduce a step-function in the underlying CCC amplitudes. Nevertheless, convergence of the  $E/2$  amplitudes to half the true ones has been achieved to a reasonable accuracy. The agreement with the measured and the DS3C-calculated spin asymmetries presented by Streun *et al* (1999) is very good. Thus the spin asymmetry experiment is unable to establish the relative accuracy of the CCC and DS3C theories. However, the DS3C and CCC TDCS are very different, particularly at the equal energy-sharing point where the CCC result is fully ab initio. Accordingly, absolute determination of the ionization cross sections, preferably as a function of secondary energy would be very welcome.

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